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A Simple Model of Photon Transport

by

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Overview

In this paper I describe a simple model of photon transport. This simple model includes: tabulated cross sections and average expected energy losses for all elements between hydrogen (Z = 1) and fermium (Z = 100) over the energy range 10 eV to 1 GeV, simple models to analytically describe coherent and incoherent scattering, and a simple model to describe fluorescence. This is all of the data that is required to perform photon transport calculations.

Each of these simple models is first described in detail. Then example results are presented to illustrate the accuracy and importance of each model.

These models have now been implemented in the Epic (Electron Photon Interaction Code). All of the figures and results presented here are from Epicshow, an interactive program to allow access to the Epic data bases, and Epicp, a simple photon transport code designed to develop optimum algorithms for later use in Epic. Epicp is made up of four parts: 1) a simple unoptimized driver to perform transport calculations, 2) an i/o package to handling reading of the binary, random access data files, 3) a physics package to handle kinematics of all processes, 4) a utility package containing all computer dependent routines, e.g., define running time, initialize random number sequence, etc. The focus is on optimizing parts 2) and 3) for later use in Epic; these are the parts that are of general interest, since they can be used in any photon transport code. Epicshow and Epicp and the Epic data bases are now available from the author.

Treatment of Integral Parameters

In this section, I discuss the treatment of integral parameters, which includes: total photoelectric, coherent and incoherent scattering, pair and triplet production cross sections, photoelectric

subshell cross sections, and expected energy deposition for photoelectric, incoherent scattering, pair and triplet production.

The data used is based on the Livermore Evaluated Photon Data Library (EPDL), which includes data for all elements between hydrogen (Z = 1) and fermium (Z = 100), over the energy range 10 eV to 100 GeV[1]. This data has been adopted as the ENDF/B-VI Photon Interaction Library [2], but at the request of the Cross Section Evaluation Working Group (CSEWG), the ENDF/B-VI data has been restricted to the energy range 10 eV to 100 MeV.

In addition to the basic integral cross sections describing coherent, incoherent, photoelectric, pair and triplet production, EPDL also includes photoelectric cross sections for each atomic subshell and expected energy deposits for each process. EPDL also includes form factors and scattering functions to describe coherent and incoherent scattering, respectively. The ENDF/B-VI library includes the photoelectric subshell cross sections, form factors and scattering functions, but not expected energy deposits (there are no ENDF/B formats for these quantities).

In evaluating the EPDL data, each physical process for each element was considered separately. The result is data represented on a different energy grid for each process and each element and generally requiring log-log interpolation between the tabulated results. Using this data in this form in applications would be extremely cumbersome, very expensive and simply not practical.

For use in applications the data has been reduced to simple tabulated form. For each element, all cross sections and average expected energy deposits are all in a simple tabulated form where all parameters are tabulated at the same energies and the tabulated energy points have been selected to allow linear interpolation to any energy between any two tabulated points. At the request of users, the energy range has been extended from the ENDF/B-VI upper limit of 100 MeV, up to 1 GeV.

Table 1 illustrates the Epic photon cross sections for lead in exactly the simple tabulated form that they are distributed. The first line defines Z, the number of tabulated points, the atomic weight and STP density of the element, and the chemical symbol. The second line identifies each column that follows: energy in MeV, six cross sections in barns, expected energy deposit per collision in MeV(note, the photoelectric energy deposit is the incident energy minus fluorescence energy = what is considered to be deposited locally). There are 100 such tables, one after the other for Z = 1 through 100. There is a similar file of data for the subshell cross sections, form factor and scattering function parameters, and fluorescence yields. For use in applications, all of these files are combined into a single binary, random access file.

The systematic variation of the photoelectric edges as a function of atomic number (Z) does not allow the data for all of the elements to be accurately represented on a common energy grid for all elements. This point will be discussed below.

Once the data for each element has been reduced to the simple tabulated form, described above, where all parameters are represented on exactly the same energy grid, and can be accurately represented using linear interpolation between tabulated points, a very efficient and almost trivial binary search can be used to define the tabulated energy interval within which the current energy

lies. Once this is done, ALL of the parameters for an element can be defined as a simple weighted sum of the contributions from the two tabulated values at the end of the interval. For example, assume that the current energy, E, lies between the tabulated energies, E_{j-1} and E_j. If we define the weights,

$$\begin{aligned} Weight_J &= \left[E - E_{j-1}\right] / \left[E_j - E_{j-1}\right] \\ Weight_{j-1} &= 1 - Weight_j \end{aligned} \tag{1}$$

then ANY and ALL parameters can be defined at energy, E, as,

$$F(E) = Weight_j * F_j + Weight_{j-1} * F_{j-1} \quad (2)$$

where F is any parameter of interest, e.g., photoelectric or pair production cross section, incoherent or photoelectric energy deposit, K or L1 photoelectric subshell cross section, etc. and F_{j-1}, and F_j are the tabulated values of F at E_{j-1} and E_j, respectively.

To represent all of the data over the entire energy range from 10 eV up to 1 GeV and allow accurate linear interpolation between tabulated points requires no more than 255 points for any given element. In creating the files, no attempt was made to keep the number of points under this limit; it just happened naturally. But the result is obviously ideal for facilitating a quick and efficient binary search.

Formerly, people have attempted to fit the photon interaction cross sections to analytical expressions that could be used in applications. This approach worked quite well to represent the basic cross sections and has been very successfully used in the past.

If we wish to perform more detailed photon transport calculations where we require more detailed information, such as photoelectric subshell cross sections, over more extended energy ranges, the approach of using analytical expressions becomes impractical.

In the case of the approach used here, a combination of 19 different cross sections and energy depositions can ALL be defined at any given energy as this simple weighted average of two tabulated terms. If one attempted to fit all of this data to analytical expressions and then had to evaluate each of the analytical expressions at each energy during a transport calculation, it seems clear which approach would be both faster and more accurate, i.e., the old approach of using analytical expressions simply is not practical to use for more detailed calculations.

Photon Scattering

In the following sections, discussing photon scattering, we will only be interested in developing methods to efficiently sample the normalized scattering distributions. We assume that the cross section for each process has already been defined and what we are interested in is: given that a coherent or incoherent scattering event has occurred (based on the cross sections), what is the angular, and in the case of incoherent also the energy, distribution of the scattered photons.

Below, we will see that based on the equations describing coherent and incoherent scattering, the most "natural" angular variable to use is neither angle nor cos, but rather 1 - cos; and more generally E^2 (1 - cos), where cos is the cosine of the photon scattering angle.

Coherent Scattering

The angular distribution of coherently scattered photons is a product of Rayleigh scattering and a correction factor,

sig(cos) = R(cos)*f(E,cos)

R(cos) = Rayleigh scattering

f(E,cos) = correction factor

E = incident photon energy

cos = photon scattering cosine

$$R(\cos) = [\cos^2 + 1]$$
$$= [2 - x * (2 - x)], x = 1 - \cos$$

$$f(E,\cos) = [FF(E,\cos) + AS(E)]^2 \quad (4)$$

FF(E,cos) = the Form Factor

AS(E) = the Anomalous Scattering Factor

The anomalous scattering factor plays an important role by creating minima in the coherent scattering cross section just below photoelectric edges and in causing the coherent scattering cross section to approach zero as E^2 as energy approaches zero [3].

It plays a less important role in that it effects the angular distribution of coherently scattered photons near photoelectric edges.

The important effect of the anomalous scattering factor on the coherent cross section has been included in the EPDL cross sections. The less important effect of the anomalous scattering factor on the angular distributions near photoelectric edges will be ignored here; so that we assume,

$$f(E,\cos) = FF(E,\cos^2) = Form\ Factor\ squared \quad (5)$$

Generally for use in applications, the form factor is represented in tabulated form that is then fit by some procedure (e.g., cubic spline) and sampled.

Here we will use an analytical expression that is simpler and more efficient to sample.

For a hydrogen atom the form factor is [4],

$$FF(E,\cos) = Z / [1 + B * x]^2, x = \mathrm{E}^2 * (1 - \cos) \quad (6)$$

For more complicated atoms, the form factor can be represented by a sum of terms, with each term corresponding to the contribution of each atom subshell, j,

$$FF(E,\cos) = \sum_j Aj / [1 + Bj * x]^{Nj} \quad (7)$$

so that the form factor squared, that we need for use in applications, can be represented in the form,

$$FF^2(E,\cos) = \sum_j Aj / [1 + Bj * x]^{Nj} \quad \sum_k Ak / [1 + Bk * x]^{Nk} \quad (8)$$

This form is judged to be too complicated and expensive to use in Monte Carlo calculations. So we will use the pragmatic approach of representing the form factor in the form,

$$FF(E,\cos)^2 = \sum_j Aj / [1 + Bj * x]^N \quad (9)$$

and use Aj, Bj and N as free parameters to fit tabulated form factors. N is easily defined by examining the high energy shape of the form factor, where,

Bj*x >> 1

in which case the shape is given by,

$$\sum_j Aj / [Bj * x]^N = C / [x]^N, where\ C = \sum_j Aj / Bj^N \quad (10)$$

so that N is merely the high energy log slope of the form factor. Aj and Bj are then defined to obtain the best fit to the form factor.

In the normally used definition of the form factor, it varies from Z at low energy to 0 at high energy. Since here we are fitting the square of the form factor, the one constraint that we have is,

$$Z^2 = \sum_j Aj \quad (11)$$

It has been found that the tabulated EPDL form factors can be very accurately fit using no more than a sum of three terms. For hydrogen and helium where we only have one atomic shell (K), only one term is required. For Z = 3 To 10, we have K and L shells, and only two terms are required. For higher Z elements more terms are required as the effect of each subshell can be seen. However, since generally coherent scattering is described as an interaction between a photon and the inner most, most tightly bound electrons of an atom we do not see a sum corresponding to

contributions from each subshell; the sum seems to saturate and involve contributions from only up to three discernible terms. The power N varies smoothly from 4 for hydrogen(Z = 1) to about 2.43 for fermium (Z = 100).

Figs. 1 and 2 illustrate comparisons between the original EPDL form factors and the fits that can be used in applications. These figures illustrate results for elements across the periodic table, Z = 1, 10, 20, 30, 40, 60, 80 and 100. The results indicate that these simple fits can be used to approximate the square of the form factor over ten to twelve decades of variation, i.e., well beyond the range that we can normally statistically sample.

As can be seen from these figures, at low energy the form factor is virtually isotropic and sampling only involves sampling the Rayleigh cross section. However, at higher energies the form factors are very strongly forward peaked and dominate the definition of the angular distribution of coherently scattered photons.

This suggests using a rejection technique to first analytically sample the form factor and then accept or reject based on the Rayleigh cross section.

The integral of each term of our fit is,

$$P = \int_0^y Aj * dy' / [1 + Bj * E^2 * y']^N \tag{12}$$
$$= \left[Aj / (Bj * E^2)\right] * \left\{1 - 1 / [1 + Bj * E^2 * y]^{N-1}\right\} / (N - 1)$$

$$= \frac{Aj * \left[(1 + Bj * E^2 * y)^{N-1} - 1\right]}{(N-1) * Bj * E^2 * \left[(1 + Bj * E^2 * y)^{N-1}\right]} \tag{13}$$

The normalization is defined by setting y = 1 - cos = 2,

$$= \frac{Aj * \left[(1 + Bj * E^2 * 2)^{N-1} - 1\right]}{(N-1) * Bj * E^2 * \left[(1 + Bj * E^2 * 2)^{N-1}\right]} \tag{14}$$

The normalization can be calculated in advance for each of the terms of the fit as a function of incident energy at the same energies at which the cross sections are tabulated. Then when a coherent scatter occurs, the tabulated normalization can be used to quickly randomly select one of the three terms based on its normalization, i.e., its contribution to the sum of terms.

From this point on, we need only be concerned with randomly sampling the one term of the series that we have selected. The normalized form for one term is,

$$= \frac{\left[Aj/\left(Bj*E^2\right)\right]*\left\{1-1/\left[1+Bj*E^2*y\right]^{N-1}\right\}/(N-1)}{\left[Aj/\left(Bj*E^2\right)\right]*\left\{1-1/\left[1+Bj*E^2*2\right]^{N-1}\right\}/(N-1)} \tag{15}$$

$$= \frac{\left\{1-1/\left[1+Bj*E^2*y\right]^{N-1}\right\}}{\left\{1-1/\left[1+Bj*E^2*2\right]^{N-1}\right\}} \tag{16}$$

$$P = \frac{\left\{1-1/\left[1+Bj*E^2*y\right]^{N-1}\right\}}{\left\{1-1/\left[1+Bj*E^2*2\right]^{N-1}\right\}},\ P\ =\ a\ random\ number,\ 0\ to\ 1 \tag{17}$$

The scattering angle is then defined by analytically inverting and solving for y (y = 1 - cos),

$$\begin{aligned} &Define,\ Q = Bj*E^2 \\ &\qquad D = 1+2*Q \\ &\qquad E = 1+y*Q \\ &\qquad C = 1/\left[1-1/D^{N-1}\right] \end{aligned} \tag{18}$$

$$\mathrm{P} = \left\{1-1/E^{N-1}\right\}\left\{1-1/D^{N-1}\right\}$$

$$\left[1-1/D^{N-1}\right]*P = 1-1/E^{N-1}$$

Inverting and solving for y,

$$y = \frac{\left\{D-\left[P+(1-P)*D^{N-1}\right]^{\left[1/(\mathrm{N\text{-}1})\right]}\right\}}{Q*\left[P+(1-P)^{N-1}\right]^{\left[1/(\mathrm{N\text{-}1})\right]}} \tag{19}$$

The above equations may seem complicated, but the entire sampling only involves, select a random number P, and then define,

$$
\begin{aligned}
&Q = Bj * E^2 \\
&D = 1 + 2 * Q \\
&F = \left[P + (1-P) * D^{N-1}\right]^{\left[1/(N-1)\right]} \\
&y = [D - F]/[Q * F]
\end{aligned}
\tag{20}
$$

The two limits of P = 0 and P = 1 can be easily seen to correspond to,

$$
\begin{aligned}
&P = 0 \\
&F = D \\
&y = [D - D]/[Q * D] \quad = 0 \quad = 1 \; - \; \cos,\ \cos = +1
\end{aligned}
\tag{21}
$$

$$
\begin{aligned}
&P = 1 \\
&F = 1 \\
&y = [D - 1]/\ Q = 2 * Q\ /\ Q = 2 = 1 - \cos,\ \cos \ = \ -1
\end{aligned}
\tag{22}
$$

At low energy, where,

$$
\begin{aligned}
&Q = Bj * E^2 << 1 \\
&D = 1 + 2 * Q
\end{aligned}
$$

We can expand terms,

$$
D^{N-1} \qquad \sim 1 + 2 * (N-1) * Q \tag{24}
$$

$$
\begin{aligned}
P + (1-P) * D^{N-1} \qquad &\sim P + (1-P) * \left[1 + 2 * (N-1) * Q\right] \\
&\sim 1 + (1-P) * 2 * (N-1) * Q
\end{aligned}
\tag{25}
$$

$$
\left[P + (1-P) * D^{N-1}\right]^{\left[1/(\mathrm{N}\text{-}1)\right]} \qquad \sim 1 + (1-P) * 2 * Q \tag{26}
$$

$$D - \left[P + (1-P) * D^{N-1}\right]^{\left[1/N-1\right]} \sim 1 + 2 * Q - \left[1 + (1-P) * 2 * Q\right]$$
$$\sim 2 * Q * \left[1 - (1-P)\right] \quad (27)$$
$$\sim 2 * Q * P$$

$$y \sim 2 * Q * P / \left\{Q * \left[1 + (1-P) * 2 * Q\right]\right\}$$
$$\sim 2 * P / \left[1 + (1-P) * 2 * Q\right] \quad (28)$$

almost isotropic (the 2*P term in the numerator) with a presumably small correction term in the denominator (presumably small, since we assumed Q << 1).

Lastly accept or reject based on the Rayleigh cross section; an energy independent efficiency of 66% (i.e., 2/3).

Incoherent Scattering

The angular distribution of incoherently scattered photons is a product of the scattering function and the Klein-Nishina formula,

$$sig(\cos) = SF(E, \cos) * KN(E, \cos) \quad (29)$$

SF(E,cos) = the scattering function
KN(E,cos) = Klein-Nishina formula

$$= C * (A'/A)^2 * \left[A/A' + A'/A - 1 + \cos^2\right]$$
$$= C * (A'/A)^2 * \left[\left(1 + \cos^2\right) + (A/A' + A'/A - 2)\right] \quad (30)$$
$$= C * (A'/A)^3 * \left[\left(1 + \cos^2\right) * (A/A') + (A/A') * (A/A' + A'/A - 2)\right]$$

A = photon incident energy in electron rest mass units.

The energy of the scattered photon is,

$$A' = A/[1 + A * x], x = 1 - \cos \quad (31)$$

Substituting for A' and canceling terms we find,

$$KN(E,\cos) = \frac{\left[1+\cos^2\right]\left[1+A*x\right]+\left[A*x\right]^2}{\left[1+A*x\right]^3} \tag{32}$$

$$= \frac{\left[2-x*(2-x)\right]*\left[1+A*x\right]+\left[A*x\right]^2}{\left[1+A*x\right]^3} \quad , x = 1-\cos$$

Note, at low energy as A approaches zero, the Klein-Nishina equation approaches Rayleigh scattering,

$$KN(E,\cos) \rightarrow \left[1+\cos^2\right] \tag{33}$$

and the energy of the scattered photon approaches that of the incident photon, i.e., the energy loss approaches zero and incoherent scattering approaches coherent scattering.

As in the case of coherent scattering, we will use an analytical expression to represent the scattering function. For hydrogen we have the relationship,

$$SF(E,\cos) + FF(E,\cos)^2 = 1 \tag{34}$$

Although this is strictly not valid for other elements it is often used as an approximation. However, this suggests using,

$$SF(E,\cos) = Z - FF' \tag{35}$$

where FF' has the same functional form as our fit for the form factor squared,

$$FF' = \sum_j Aj / \left[1+Bj*x\right]^N \tag{36}$$

For each element we will use the same value of N as previously defined for the form factor squared, and Aj and Bj will be treated as fitting parameters. Note Aj and Bj here need not be the same as those defined for coherent scattering, e.g., for coherent scattering the sum of the Aj is Z^2, whereas here it is Z. However, when rescaled for this difference, they are very similar as predicted by equations 34 and 35; for hydrogen they are virtually identical.

At low energy the scattering function approaches zero as E^2 in the forward direction and at high energies it approaches unity in the backward direction; indeed in almost all directions, except the extreme forward direction.

For the normally used definition of the scattering function, it varies from 0 at low energy to Z at high energy. Therefore the one constraint that we have is,

$$Z = \sum_j Aj \tag{37}$$

and we can write,

$$
\begin{aligned}
SF(E,COS) &= Z - \sum_j Aj / \left[1 + Bj * x\right]^N \Big\} \\
&= \sum_j \left\{Aj - Aj / \left[1 + Bj * x\right]^N \right\} \\
&= \sum_j Aj * \left\{\left[1 + Bj * x\right]^N - 1\right\} / \left[1 + Bj * x\right]^N
\end{aligned}
\tag{38}
$$

The results are similar to those obtained for coherent scattering, in the sense that it has been found that in no case are more then three terms required to obtain excellent agreement between the EPDL scattering functions and the fit. One term is adequate for Z = 1 or 2, where we only have one shell (K). Two terms are required for Z = 3 to 10, where we have two shells (K, L). Higher Z elements require an additional term. Incoherent scattering is usually described as an interaction between a photon and the outer most, most loosely bound electrons. So what we seem to see is that the sum rather than including contributions from each subshell, saturates and only requires up to three terms to represent the contribution of the outer most subshells.

Figs. 3 and 4 illustrate comparisons between the original EPDL scattering functions and the fits that can be used in applications.

At low energies the scattering function plays an important role in suppressing forward scattering, compared to the Klein-Nishina formula. In the case of extreme low energies it essentially multiplies the Klein-Nishina formula by E^2. At higher energies the scattering function plays very little role, except at very forward angles where it will always suppress the forward scattering. At very high energies it plays essentially no role and is often simply ignored in applications.

This suggests using a rejection technique to first sample the Klein-Nishina formula and then accept or reject based on our fit. In this case we need not invert our fit (as was done in the case of coherent scattering), we merely first sample the Klein-Nishina formula to define x and then define the sum,

$$
SF(E,\cos) = \sum_j Aj * \left\{1 - 1 / \left[1 + Bj * x\right]^N \right\} \tag{39}
$$

and accept if the sum is greater than or equal to Z times a random number. The efficiency will vary from 1/3 at low energy to essentially 1 (100% acceptance) at high energies.

Fluorescence

The Livermore Evaluation Atomic Data Library (EADL) contains data to describe the relaxation of atoms back to neutrality after they are ionized, regardless of what physical process ionized the atom, e.g., photoelectric, electron ionization, internal conversion, etc.

The data in EADL includes the radiative and non-radiative transition probabilities for each subshell of each element, for Z =1 through 100. Given that an atom has been ionized by some process that has caused an electron to be ejected from an atom, leaving a “hole” in a given

subshell, the EADL data can be used to calculate the complete radiative (fluorescence) and non-radiative (Auger and Coster-Kronig) spectrum of x-rays and electrons emitted as the atom relaxes back to neutrality [6].

For a K shell photoelectric event in uranium if fluorescence is not considered all of the energy of the photon is assumed to be deposited locally, at the point of the event. If fluorescence is considered, a portion of the approximately 116 keV binding energy of the ejected electron will be emitted as fluorescence x-rays. The portion emitted will be independent of the photons incident energy, i.e., every photoelectric event leads to an ionized atom that will then return to neutrality, independent of how it was ionized.

Figs. 5 and 6 illustrate that these spectra can be quite complex. In this case a single "hole" in the K shell of uranium statistically leads to the emission of 154 different energy x-rays and 2772 different energy electrons. Of course in any single given event far fewer x-rays and electrons are emitted, but when averaged over a large number of such events this will be the observed emitted spectra. The most important point to note is that rather than the entire energy being deposited locally, over 89% of the binding energy is re-emitted as fluorescence x-rays. These x-rays are emitted just below photoelectric edges, where the cross sections an be quite small, which allows these x-rays to be quite penetrating. In absolute terms this means that a photoelectric event due to a photon just above the K edge at 116 keV will lead to the emission of about 100 keV of fluorescence x-rays - 89% of its energy; a 1 MeV photon will also result in about 100 keV of fluorescence x-rays - about 10% of its energy, etc. In the case of a 116 keV photon the local deposition will only be 16 keV. However, if fluorescence is not considered, it is assumed to be 116 keV; over 700% higher than the actual value. This over estimation will decrease at higher energies, but even by 1 MeV it will still be about 10% too high. From Fig. 5 we can see that most of the fluorescence x-ray energy will be emitted in a narrow band near 100 keV, just below the K edge where the cross section is only about 25% of the cross section at the top of the K edge, allowing these x-rays to be quite penetrating. For photon transport calculations extending down to energies below several MeV, to realistically model the transport, these fluorescence x-rays should be included in calculations.

This point has been recognized for many years and fluorescence has been included in modern Monte Carlo photon transport codes [7, 8]. In these codes the "jump" in the photoelectric cross sections across an edge is used to estimate the fluorescence yield for each subshell.

Now that the photoelectric subshell cross sections are available from EPDL and the fluorescence yield is available from EADL we can use a more detailed model for fluorescence. The subshell cross sections can be used to define what subshell was ionized, and once a subshell is selected our fluorescence yield data can be used to define the emitted x-rays. However, to be able to do this efficiently in calculations we must decide what is or is not important and try to include only those details that are important.

These spectra are judged to be too complicated to sample in detail in applications. However, the most important details can be efficiently sampled. We can use the fact that fluorescence decreases by roughly an order of magnitude for each successive shell. For example, in the case of uranium the fluorescence due to a K shell vacancy is almost 100%, whereas the L shell will be about 10%,

the M shell about 1%, etc. In addition we can divide the photon spectrum into those x-rays due to the initial vacancy being filled (what I will refer to as direct or primary x-rays) which are the most energetic x-rays emitted, and those x-rays due to vacancies generated in other shells as the atom relaxes back to neutrality (what I will refer to as secondary x-rays). I will refer to the combination of direct or primary and secondary as the enhanced or total yield.

Fig. 5 illustrates the emitted x-rays (fluorescence) due to a single vacancy in the K shell of uranium. The boxes represent the individual emissions and the solid line represents the integral of the emitted energy spectrum. From this figure we can see that there are 154 individual x-rays emitted, but most of the emissions in terms of probability and energy are in two narrow energy bands just below the K and L edges; these two bands correspond to the direct and secondary fluorescence yields. Based on the integral of the spectrum, in this case the primary fluorescence just below the K edge accounts for about 95% of the emitted x-ray energy and the secondary emission just below the L edge another 4.8%. The entire remainder of the spectrum accounts for only about 0.2% of the emitted x-ray energy, which is small compared to the uncertainty in the emitted spectrum. This suggests that for use in applications rather than attempting to model the entire emitted fluorescence x-ray spectrum all we need model are the two narrow bands of emission just below the K and L edges, in the case of a K shell vacancy; or L and M, for L vacancies; M and N, for M vacancies, etc.

Based on the EADL data, we can calculate [6] the direct and secondary fluorescence yields, both in terms of number of photons and energy emitted as fluorescence for every subshell of every atom (Z =1 through 100). For use in calculations, this data has been reduced to a form where a vacancy in any subshell can result in the emission of up to two fluorescence x-rays where the emission probabilities and energies have been defined to exactly conserve the direct and enhanced fluorescence yields, both in terms of number and energy. These two x-rays per vacancy can accurately model the two narrow bands of emitted x-rays just below the K and L edges that we saw in the Fig. 5.

Since the fluorescence yield decreases rapidly with subshell, an accurate model of fluorescence yield does not require all of the individual subshells to be represented. For use in applications the photoelectric subshell cross sections have been grouped in: K, L1, L2, L3, M, N, O, P, Q, i.e., the most important inner subshells of K and L are represented separately, and the remaining subshells of each shell are grouped together. Furthermore, fluorescence is only considered for K, L1, L2, L3, M and N, which tracks the yield down to a very low level, well below the uncertainty in our atomic relaxation data.

Following each photoelectric event we first use the subshell cross sections to randomly select an electron vacancy in a subshell. Once this has been done, the probability of fluorescence yield for that subshell is used to randomly emit x-rays of a given energy; up to two x-rays per primary vacancy are allowed. Even in the extreme case of high Z elements where the K shell fluorescence yield can approach 100%, the two x-rays allowed in this model will track the yield from K shell vacancies down to about 1%. By allowing individual subshells to be sampled the fluorescence will be tracked down ever further in energy, e.g., if we had statistically sampled a vacancy in an L subshell the yields could approach about 10% and 1%, tracking the yield down to about 0.1%.

Pair and Triplet Production

In the case of pair production, the photon interacts with the field of an entire atom. The photon disappears and an electron-positron pair is created. The sum of the energies of the electron-positron pair is the incident energy of the photon minus the rest mass of the electron-positron pair.

In the case of triplet production the photon interacts with the field of an electron. The photon disappears and an electron-positron pair is created, and an electron is ejected from the atom (leaving an ionized atom). The sum of the energies of the electron-positron pair plus the ejected electron is the incident energy of the photon minus the rest mass of the electron-positron pair and the binding energy of the ejected electron. Compared to the energies of the electron-positron pair, generally the energy of the ejected electron is quite small.

Pair and triplet production are fairly complicated processes, since they are three body processes. For example, in pair production the electron and positron need not equally share the available kinetic energy; indeed at higher energies the spectrum for both becomes quite wide. Here I will merely mention that this spread in the spectra will effect bremsstrahlung emitted by the electron and positron as they slow down in the medium.

Here I will use the simplest possible model for pair and triplet production. I will assume that the electron and positron both slow down and come to rest close to the point of the pair or triplet production event. Therefore, all of their kinetic energy will be deposited locally, and when the positron annihilates two 0.511 MeV photons are created at the point of the pair or triplet event. In the case of triplet production, I will also ignore the low energy ejected electron and the ionized atom.

Later in this paper, I will again discuss pair and triplet under the section What's Next?

The Importance of Each Process

Fig, 7 illustrates the photon cross sections for four elements spaced across the periodic table. In all cases the variation of the cross sections are smooth functions of Z, so that even from merely these four examples we can see all of the trends of the various cross sections. This figure was produced interactively using Epicshow; the top of the figure shows the Epicshow mouse driven interactive user interface.

Generally, at low energy photoelectric is by far the dominant process. In comparison, the coherent and incoherent cross sections are so much smaller that they are of importance only in special calculations, such as back scattering measurements, where their cross sections may be small, but these are the only processes available to back scatter photons. As described above, at low energy incoherent scattering approaches coherent scattering (no energy loss) and photoelectric is the only effective energy loss process for photons.

At low energies, in high Z elements, fluorescence can be a very important effect, since it can effectively transfer photons from energies above photoelectric edges, where the cross section is

high, to energies just below the edges, where the cross section can be much smaller; thereby, allowing these photons to be much more penetrating. Since at low energies the photoelectric cross section can be very large, fluorescence can appear almost to be a surface effect, i.e., most of the photoelectric events above the edges will occur very close to the surface of a high Z element. This will tend to increase the reflection from high Z elements. However, it can also contribute to penetration through materials. For example, in high Z elements the cross section at the bottom of the K edge is about 1/4 to 1/5 that of the cross section at the top of the edge. Therefore, if we have a material that based on the cross section at the top of the K edge is say 10 mean free paths thick (we expect little if any transmission), fluorescence can move photons to below the K edge where the cross section is only 2 to 2.5 mean free paths thick.

At high energies pair and triplet production become the dominant processes. Above about 10 MeV their cross sections are so much larger than the coherent and photoelectric cross sections that the latter can be effectively ignored. Even at fairly high energies incoherent scattering continues to play an important role and should not be ignored. At these high energies coherent and incoherent scattering are very forward peaked, and cause very little back scatter.

At intermediate energies between the high keV and low MeV regions incoherent scattering can be very important. In this energy range the photoelectric cross section has decreased to a small value and the pair and triplet production cross sections have not yet become significant. Therefore, the only effective process that can decrease the energy of photons is incoherent scattering. From Fig. 7 we can see that incoherent scattering in this energy range is particularly important for low Z elements, e.g., hydrogen. At lower energies the incoherent cross section approaches zero as E^2, and becomes dominated by the rapidly increasing photoelectric. Similarly, at higher energies the incoherent cross section decreases, and eventually becomes dominated by the rapidly increasing pair and triplet production cross sections.

Coherent scattering can be an important process in the keV region, in that by scattering photons it will tend to keep them from escaping from a medium, but in no case is coherent scattering the dominant process. At lower energies the coherent cross section approaches zero as E^2, and at higher energies it also decreases toward zero. Just below photoelectric edges in high Z elements the coherent cross section can be a significant contribution to the total cross section, e.g., about 10%, that does effect transport.

Example Results

All of the data discussed above is now available in a simple tabulated format, to allow the data to be easily moved between computers. On any given computer it is then converted to binary, random access files for use in applications. This data can be examined using the program Epicshow [9] and photon Monte Carlo transport calculations can be performed using program Epicp [10].

Epicp is designed as a test bed program to develop optimum algorithms for handling photons, for later use in Epic (Electron Photon Interaction Code). Epicp uses all of the data described in this report, and allows various models to be turned on or off, to determine the importance of each model. For example, coherent and incoherent scattering can be modeled either with or without

form factors and scattering functions. Photoelectric events can be modeled with or without fluorescence emission. Cross sections can be modeled using the energies at which they are tabulated in the data bases (most accurate) or using the same fixed energy grid for all elements (fastest). By comparing the results and running time using different models we can easily determine how accurate any given model is and how expensive it is to use. All of the example results presented below were calculated using Epicp.

Below, I present results to illustrate the use of this data and I also present conclusions that can be reached from these results. In all cases I will use a simple geometry, so that we can easily interpret the results. I will use cylindrical geometry to simulate a detector, and I will calculate: 1) deposition within the detector, 2) transmission through the detector, 3) reflection from the detector, and 4) lateral leakage from the detector. No attempt has been made to fold the results with a detector response function; the results presented are exactly as calculated, and therefore differ from what one would actually measure with a real detector. This has been done intentionally in order to emphasize the effects that will be discussed below.

For additional details of the examples presented below and additional examples see the report on program Epicp, reference 10.

Detector Response and Leakage

In order to correctly interpret the results presented below the reader must understand the definitions of detector response and leakage used here. Starting from each source photon Epicp tracks this photon and all photons that it may produce (through pair production, fluorescence, etc.) until they have all "disappeared", i.e., either leak or are absorbed. For each source photon this is defined to be one history. The detector response is then defined as one count, corresponding to the total energy deposited in the detector during the entire history. Since Epicp only tracks photons, it is assumed that everything happens at the speed of light and rather than responding separately to each event that occurs within the detector, the detector will add all of the energy deposited by all events during a history and score a single count corresponding to the total energy deposited during the entire history.

For example, consider the typical history of a 10 MeV photon incident on the detector. Assume the initial photon undergoes pair production. The result will be a deposition of the incident energy of the photon minus the energy of two 0.511 MeV photons produced when the positron annihilates, but the history isn't finished yet. Each of the 0.511 MeV photons is then separately tracked. Each may undergo more collisions and deposit all or a portion of their energy, or they may leak from the detector. Let's consider the energy deposited for three cases: 1) both 0.511 MeV photons are absorbed in the detector = all 10 MeV of the incident photon is deposited, 2) one 0.511 MeV photon leaks = about 9.5 MeV is deposited, 3) both 0.511 MeV photons leak = about 9 MeV is deposited. In each of these cases the total amount of energy deposited is recorded as a single event, so that these three cases correspond to three different energy depositions of about 10, 9.5 or 9 MeV.

In contrast Epicp defines transmission, reflection and lateral leakage for each event separately. In the above example the leakage for the three cases is: 1) no leakage, since everything was absorbed in the detector, 2) one 0.511 MeV photon leaked, 3) two 0.511 MeV photons leaked. It is

important for the reader to understand the difference between how deposition and leakage are defined here. In case 3 the deposition will have a single score about 1 MeV below the source energy, whereas the leakage will have two scores at about 0.5 MeV - not one score at about 1 MeV. Therefore in contrast to deposition where there are three different depositions about 0, 0.5 or 1.0 MeV below the source energy, the leakage will only include either 0, 1 or 2 scores all at about 0.5 MeV.

When leakage occurs (transmission, reflection or lateral leakage) each event is scored as one count, without any consideration of the direction of leakage. This corresponds to scoring the first, not zeroth, angular moment of the photon distribution. To score the zeroth angular moment of the photon distribution each event should be weighted by the reciprocal of its direction cosine relative to the normal of the surface it crosses. Therefore the leakage as defined here corresponds to the source of photons that one would see leaking from the detector.

The definition of deposition used here is designed to correspond to what we would really see when performing an experimental measurement; except that the effects of electron and positron transport and the actual response of the detector's electronics have not been included. As we incorporate more sophisticated models into the calculation this will allow us to use the many published experimentally measured detector responses to benchmark our calculations.

The definition of leakage used here is designed to provide us with as much information as possible to understand what is physically happening. For example, in order to conserve energy all of the energy incident on the detector must either be deposited within the detector or leak from it. Therefore if Epicp defined leakage in exactly the same way it defines deposition we would end up with two completely complementary distributions that do not provide much more information than just one of these distributions. In contrast, with the definition of leakage used here we can obtain additional information about individual events. For example, for any given history additional photons may be produced and there can be leakage events corresponding to transmission, reflection and lateral leakage - all due to only one history. By scoring each of these separately we can obtain additional information. This may not correspond to anything that can actually be measured with a real detector (which would add together all events from each history), which is all right since this is not what the leakage as defined here is intended to be used for. Here the leakage is defined to provide us with more insight into what is physically happening.

Even though Epicp is primarily designed to perform detector response calculations in cylindrical geometry, it can also be used to calculate transmission and reflection in planar geometry. In this case, as defined here the leakage corresponds to what a normal photon calculation would define as the source of photons transmitted or reflected - let me stress that this is what a transport code would calculate, not what a detector measurement would indicate (as explained above). Therefore with the definition of leakage used here the results are directly comparable to those produced by other photon transport codes, allowing us the possibility to benchmark our results against those of other codes.

High Energy Application

The first application is a monoenergetic 4.43 MeV photon incident on a NaI detector 7.62 cm in diameter and 7.62 cm in depth. This example is intended merely to introduce the idea of detector deposition and to point out one approximation that should be avoided.

Figure 8 presents Epicp results for this problem. In this case the analog and expected results have converged to the point where we cannot see any difference between them. The transmission, reflection and lateral leakage are in units of photons per MeV for each contributing individual event. In the case of deposition, for each incident photon the total amount of energy deposited is scored as a single event. If all of the energy of all incident photons is deposited the result would be non-zero only at 4.43 MeV. Instead we see a typical response function. Note, the peaks about 1 and 0.5 MeV below 4.43 MeV. These correspond to the build up and escape from the detector of both or one of the 0.511 MeV photons created by positron annihilation. The results have not been folded with the detector response in order to more clear see and understand these two peaks; in an actual detector response these peaks are much wider. The transmission, reflection, and lateral leakage all show peaks due to the leakage of 0.5 MeV photons. We do not expect a peak near 1 MeV, since even if both 0.5 MeV photons leak they are scored as two separate 0.5 MeV photons. In the deposition just above the peaks 0.511 and 1.022 MeV below the source energy we can see the effect of Compton scattering that has caused photons to lose some of their energy before leaking, thereby increasing their deposition. We see a complementary effect in the leakage just below the 0.511 MeV peak.

The continuous spectrum down to low energy seen in figure 8 is the result of Compton scatters, at the source and lower energies, in which a photon can lose (deposit) any amount of energy between zero and some maximum amount and then either scatter again or leak. The complement to this low energy tail in the deposition is the high energy tail in the transmission; photons that lose a small amount of energy have scattered through a small angle, continue transporting forward and are transmitted with a high remaining energy. Similar continuous spectra can be seen in the lateral leakage at lower energy (since the photons must scatter through larger angles to laterally leak) and at even lower energies in the reflection (the photons must scatter through at least 90 degrees).

In this case the most prominent features in the deposition are the narrow peaks due to pair production, but most of the energy deposit is due to Compton (incoherent) scattering. For each MeV of energy incident about 65% is deposited: about 40% from Compton, 21% from pair production, and 4% from photoelectric. Of the remainder about 27% is transmitted, 7% laterally leaks and less than 1% is reflected.

One might think that in this case the calculation could be sped up by assuming that rather than each pair production event leading to two separate 0.511 MeV photons, we could assume that we will run enough photons histories that we could assume that each pair production events produces only one 0.511 MeV photon, of weight 2; the large number of photon histories could then be relied on to supply enough events to adequately describe the position and direction of all such photons. This assumption actually works quite well to describe the transmission, reflection, and lateral leakage, but not the deposition. In order to reproduce the two peaks in the deposition one must track each of the photons separately, otherwise you can never have the case where only one of them escapes, leading to the peak about 0.5 MeV below the source energy. With the model used here, where it is assumed the positron comes to rest and two 0.522 MeV photons are

produced, the direction of the two photons is completely correlated; if one is moving in a given direction the other is moving in the opposite direction. If you are interested in designing a photon transport code you should consider these points.

Fixed or Variable Cross Section Energies

There are a number of Monte Carlo codes [7, 8] that use a fixed set of energies to represent all photon cross sections for all elements. This simplifies the codes and speeds up the calculation, e.g., for a photon of a given energy, once you have defined the energy interval in the cross section tables this can be used to define the cross sections for all materials in all zones.

This approach requires that certain compromises be accepted between speed and accuracy. For example, the energy of the K edge of each element is to a good approximation a simple logarithmic function of atomic number, varying from about 14 eV for hydrogen (Z = 1), to about 140 keV in fermium (Z = 100). Without using an excessive number of tabulated energy points over this energy range, it would be difficult to accurately approximate the K edge for all elements. If we consider not only the K edge, but all other edges, plus the additional general problem of accurately interpolating in energy between tabulated values, we must conclude that if we wish to use the same energies for all elements we will have to somehow compromise the accuracy of the photon cross sections. Is this important?

This effect will only be important at energies near and below K edges, i.e., in the worse case below about 150 keV. For higher energy applications, there is no problem in using the same energy points for all elements; the only point to be concerned with is properly modeling the onset of pair production at its 1.022 MeV threshold and triplet production at its 2.044 MeV threshold. Therefore, the following discussion is only of interest to those readers involved in lower energy applications.

What we will examine here is: 1) how accurate is this procedure, 2) how much faster is it than representing the cross sections for each element using a different set of tabulated energies for each element, 3) what are the real advantages of one approach versus the other.

In an attempt to answer these questions, we will use the 176 energy points used by the TART code to represent all cross sections and first see what effect this has on both the position of the K edge and the magnitude of the cross section near the K edge. The Epic cross sections model each photoelectric edge as a discontinuity with repeated energy points at the bottom and top of each edge. TART represents an edge with the two nearest fixed energy points on either side of the real edge energy. How accurate is this? We will use exactly the procedure used to make the photon data library used by TART, 1) interpolate the actual photon cross sections to the 176 energies and define the value strictly based on interpolation (no attempt is conserve integrals or anything else), 2) I will then define the "TART position of the K edge" bottom and top as the first energy at or below the actual K edge and the first energy at or above the actual K edge, 3) we can then compare the value of the cross sections at these points to the actual values in EPDL.

Fig. 9 presents results for the entire periodic table, from Z = 5 through 100 (TART only extends down to 100 eV and as such does not include the K edge of the lowest Z elements). First the

figure shows a comparison of the energy of the EPDL K edge to the TART K edge top and bottom energies. What we see, is that using the TART 176 energy points can shift the energy of the top and bottom of the K edge by about 10% for a number of elements. The figure next compares the value of the cross section at the bottom and top of the K edge for EPDL and TART. What we see is that using the TART 176 energy points can increase the bottom cross section by up to about 30% and decrease the top cross section by up to 30% for a number of elements. Lastly, the figure shows the values at both top and bottom of the K edges. From this figure we can see that the changes in the cross section due to using the TART 176 points tend to move the top and bottom values up and down together; fortunately, we do not have any cases where 30% changes move in opposite directions, thereby, changing the jump ratio across the K edge by even more.

In order to determine whether or not these changes are important, we can now use the above results to select some worst cases from the entire periodic table and see what happens in an actual transport calculation.

On the basis of the changes in the position and magnitude of the cross sections, when using a fixed energy grid, one might expect to see rather large differences in the results using one method or the other. By using a number of Epicp and TART runs focused on where we expect to see large differences, the results indicate surprisingly little difference in the results. As long as a problem involves a broad spectrum of photons, the energy intervals over which the cross sections are modified near the K edges is small compared to the entire energy range of interest and results in very little change in overall answers.

However, if the focus of the application is effects near the K, or other edges, then one can see rather large differences in the results. For example, obviously, if you decrease the photoelectric by 30% you expect a decrease in deposition by 30%, but only over the narrow energy range where the cross section was deceased. If this is the energy range of interest to you, this is an important effect. A second effect to consider, is that in shifting the K edges by up to 10%, it may no longer be possible to use transmission measurements and calculations defining the position and strength of K edges to define the composition of a material containing neighboring or near Z elements.

Figure 10 compares the fluorescence yield as a fraction of the incident photon energy using the original tabulated energies (as read from the data base), 176 and 401 fixed energy points. If you only consider a wide energy range, using fixed energies will have little effect on integral values (top of figure). For this particular problem of transport through Z = 90 (where we expect large differences) there is no significant difference in the integral deposit, transmission, reflection or lateral leakage; differences occur over such a small portion of the total energy range that the effect on integral values is simply not significant. However, if you are interested in very narrow energy ranges, particularly near edges, using fixed energies can have a significant effect (bottom of figure). In this case the fluorescence yield and therefore deposition are obviously effected, but it is also difficult to see the K edge, which makes it difficult to determine the composition of this material. Is this an important effect in your applications? Only you can answer this question.

In terms of running time, there is a definite advantage to using fixed energies. For simple problems only involving a few materials and zones, there isn't that much difference between them. However, as problems become complex and involve more and more materials and zones, using fixed energies results in significantly less running time. In the latter case, a mixture of materials decreases the importance of changes across edges, further justifying the use of fixed energies.

In terms of simplicity of the codes, there is a definite advantage to using a fixed energy grid, e.g., in complicated geometry defining the cross section when a photon enters each spatial region is much simpler using a fixed energy grid.

In summary, based on the above results, it appears that each approach can be used to good advantage in different applications, and it is not possible to make one sweeping general recommendation that one approach is "better" than the other. If you are willing to invest the time to handle different energies for each element you can be sure that your code will be quite general and need not worry about the special situations described above; be aware, you will pay a penalty in running time for complicated problems. However, if you already have a code that uses fixed energies and you do not want to invest the time to upgrade it, for most calculations involving broad spectra of photons and only considering integral response over wide energy ranges, fixed energies are adequate to obtain accurate answers.

Epic tries to accommodate both approaches. In the Epic data base each element is tabulated using energies that have been selected to best represent the data. For use in application the user has the option to perform calculations using the data exactly as represented in the data base (most accurate), or using the same, fixed energy grid for all elements (fastest). Conversion to the latter form as the data is read from the data base for use in calculations is trivial and does not add any significant overhead to calculations. As an improvement over the TART 176 point between 100 eV and 30 MeV, Epic uses 401 points between 10 eV and 1 GeV, with 50 points logarithmically equally spaced in each energy decade; this completely uniform spacing from 10 eV to 1 GeV allows the energy interval for cross section lookup to be defined using a single line of FORTRAN coding. Similar to the above results for TART (Fig. 9), Fig. 11 shows results for this 401 fixed point energy grid. From this figure we can see that the 401 points results in shifts of K edge energies by up to 4% (compared to 10% for TART), and changes in the cross section by up to 10% (compared to 30% for TART). With this approach users can select whatever scheme is most appropriate for their calculations, i.e., either accuracy or speed.

It is worth observing that there have been great improvements in the detail included in modern neutron evaluations and this detail has been included in modern Monte Carlo transport codes where cross sections for individual elements or isotopes are represented by many thousands of energy points, using different tabulated energies for each material (for example, see reference 8). In comparison it seems that the improvements in photon evaluations have not been incorporated in codes and many continue to used fixed energy grids for all materials, even though in terms of the number of tabulated energy points required, the problem of using different tabulated energies for each element for photon transport is orders of magnitude simpler than in the case of neutrons. As we extend our computer codes to treat an very expanding variety of applications in more and more detail and ask for ever improving accuracy, we should consider improving our treatment of photon data in order to insure accuracy in our results.

Fluorescence

Fluorescence yield is a function of atomic number (Z). For the K shell it varies from close to 100% for fermium (Z = 100) to essentially 0% for hydrogen (Z = 1). It is also a function of shell, decreasing by roughly a factor of 10 for each successive shell, e.g., from close to 100% for K, about 10% for L, etc. It is also a function of energy, being important only close to photoelectric edges. Therefore, we need not be concerned with low Z elements, or high energy applications, well above the K edges of all materials involved. However, we should look at high Z elements for lower energy applications, i.e., below a few MeV.

The following example illustrates the effect of fluorescence. In this example Epicp's option to turn fluorescence on or off has been used. When fluorescence is turned off, at each photoelectric event all of a photon's energy is deposited locally, at the site of the event. When fluorescence is turned on, a portion of the photon's energy can be re-emitted as fluorescence x-rays, usually just below the photoelectric edges. If these re-emitted x-rays deposit all of their energy we expect the overall deposition to be the same as when fluorescence is turned off. However, if they leak from our detector the deposition will be decreased. Therefore with fluorescence we expect the overall deposition to be equal to or less than the deposition without fluorescence. Even in the case where the overall deposition is the same, fluorescence can effect the spatial distribution of the deposition.

In the following example I will use a bremsstrahlung spectrum filtered through cadmium; see figure 12. I will use a cylindrical detector composed of the following atom fractions: 53-I, 1 atom, 55-Cs, 1 atom, 81-Tl, 0.012801 atoms, normalized to an overall density of 4.51 grams/cc. Figure 13 illustrates the cross sections for this composition and each element. The detector is 13.1072 cm in radius and 0.0111 cm thick. We expect fluorescence to be most important for high Z elements, so that this is by no means the most important case in which to consider the effect of fluorescence. However, it will serve to illustrate that fluorescence is an important effect even for elements in the middle of the periodic table.

In this case since there is essentially no lateral leakage, we need only look at the reflection, transmission and deposition to see what happened. To be able to easily interpret these results figures 14 through 16 present: 1) results with fluorescence turned on, 2) results with fluorescence turned off, 3) both results on the same figure.

Without fluorescence (see figure 15) essentially the only process that is contributing anything is photoelectric and what we see is simple exponential attenuation of the incident source spectrum according to the strength of the source and the magnitude of the cross section at each energy.

With fluorescence the results are quite different. In this case by comparing the two results (see figures 14 through 16) we can see that with fluorescence the deposition at higher energies (~ 35-50 keV) is significantly less than without fluorescence. In addition, with fluorescence we see a peak in the deposition in the ~ 5-20 keV range that simply doesn't exist in the results without fluorescence. We can also see the narrow peaks in the reflection and transmission due to fluorescence. What the results indicate is that with fluorescence turned on, statistically in some

events fluorescence does not occur and the deposition at higher energy (~35-50 keV) is similar in shape to the results with fluorescence turned off, since both correspond to events in which no fluorescence occurred. The magnitude is suppressed in proportion to the probability of fluorescence not occurring. The second peak in the deposition in the ~ 5-20 keV range corresponds to those events in which statistically fluorescence did occur, the fluorescence x-rays leaked from the detector and the remaining energy was deposited; this is similar in shape to the ~ 35-50 keV portion of the deposition curve, merely shifted to lower energies by the amount of fluorescence energy that has leaked from the detector. Since without fluorescence this peak cannot occur it is not see in the results when fluorescence is turned off, nor is any of the other narrow sharp peaks in transmission, reflection or deposition present.

Not only are the energy dependent results different; the integral results are also quite different. With fluorescence about 43.3 % of the energy is deposited, 8.1 % reflected, and 48.5 % transmitted. When fluorescence is turned off the results change to 57.5 % deposited, 0.2 % reflected and 42.3 % transmitted. Without fluorescence at each photoelectric event all of the photon's energy is deposited (57.5 %). With fluorescence a portion of the energy is re-radiated and more energy leaks from the detector, decreasing the deposition to 43.3 %, and increasing both reflection and transmission. Note, in particular the dramatic difference in reflection: 8.1 versus 0.2 %. In this energy range the cross sections above the photoelectric edges are so large that fluorescence is almost a surface effect. A large number of photoelectric events are occurring very close to the incident surface of the detector. Fluorescence x-rays are being created at energies below the photoelectric edge where the cross section is much smaller, allowing these x-rays to leak from the detector; particularly at the nearest, reflection, surface. From figure 16 comparing results with and without fluorescence we can see that virtually all of the reflection is due to the two very narrow fluorescence lines near 28 and 31 keV.

In summary, for applications involving high Z elements, below a few MeV, it is important to include the effect of fluorescence in order to obtain realistic calculational results. At higher energies the photoelectric cross section is so small that the probability of a photoelectric event, and therefore, fluorescence is very small. Therefore, it isn't necessary to build into codes a rule of thumb to ignore fluorescence above some incident photon energy; it happens naturally based on the cross sections.

Incoherent Scattering

Fig. 17 summarizes the effect of the scattering function on the incoherent cross section. This effect is important at low energies and extends up to several hundred keV in high Z elements. Without the scattering function the incoherent cross section, defined by integrating the Klein-Nishina formula, approaches a constant value at low energy. With the scattering function it approaches the correct zero limit as E^2 at low energy. At lower energies where both coherent and incoherent cross sections are approaching zero as E^2, obviously including the effects of anomalous scattering and the scattering function, greatly reduces total scattering. Since the effect of the scattering function on the incoherent cross section has been included in the Epic incoherent cross sections, we need not explicitly consider the effect further. However, we do have to consider the effect on scattering angle and energy loss.

For Compton (incoherent) scattering, compared to only using the Klein-Nishina formula, the scattering function causes photons to scatter through larger angles and lose more energy. In the following example the same detector as described above has been used and Epicp's option to turn the scattering function on and off has also been used. When Epicp's option to turn off the scattering function is used the incoherent cross section calculated including the effect of the scattering function is still used, but the scattering function is not used to define the angular and energy distribution of scattered photons; only the Klein-Nishina formula is used. From the plot of the cross sections (see figure 13) we can see that Compton scattering is the largest cross section near 1 MeV. The following results are for monoenergetic 1 MeV photons incident on a detector 3 cm thick.

In this case there is very little difference in the total energy deposition: about 27 % is deposited due to incoherent and 11.5 % due to photoelectric. About 60 % of the energy is transmitted. The biggest difference that we see is that without the scattering function about 0.9 % of the energy is reflected and with the scattering function about 1.7 % is reflected; almost a difference of a factor of two. These results are consistent with our expectation that the scattering function will cause photons to scatter through larger angles, thereby increasing the reflection. This seems to be a small effect, but if you are interested in back scattering it can be a rather important effect for your applications.

In low Z elements the Compton cross section is dominant over a fairly large energy range (see figure 7). In the following example I consider Z=1, hydrogen, at a density of 1 gram/cc, for three different monoenergetic source energies: 1 MeV, 100 and 10 keV. I have used a large radius, so this is essentially a plane of hydrogen. In each case the detector thickness has been selected to allow roughly half the energy to be transmitted: very roughly half.

At 1 MeV, the energy results with the scattering function are: 54.2 % deposited, 10.1 % reflected and 35.7 % transmitted and without it: 55.3 % deposited, 4.5 % reflected and 40.2 % transmitted. In this case virtually all of the deposition is due to incoherent scattering. Note that with the scattering function the reflection has more than doubled. Even though each scatter with the scattering function causes photons to lose more energy, the increase in the reflection contributes to decreasing the total number of scatters in the detector, leading to the small decrease in deposition.

At 100 keV, the energy results with the scattering function are: 13.8 % deposited, 29.3 % reflected and 56.9 % transmitted and without it: 14.8 % deposited, 19.2 % reflected and 66 % transmitted. In this case incoherent scattering still contributes the majority of the deposition, but there is a small contribution from photoelectric. Compared to the 1 MeV case, in this case incoherent scattering is less effective in depositing energy.

At 10 keV, the energy results with the scattering function are: 4 % deposited, 50.4 % reflected and 45.6 % transmitted and without it: 4.4 % deposited, 32.9 % reflected and 62.7 % transmitted. The energy deposition due to Compton has now been drastically reduced, because at progressively lower energies Compton becomes a progressively less effective process for losing energy. The maximum energy loss per photon collision is roughly: 1 keV ~ 0.4%, 10 keV ~ 4%, 100 keV ~ 28%, 1 MeV ~ 80%. Even though at lower energies incoherent scattering does not deposit much energy, at lower energies the scattering function will tend to make the photons

scatter through larger angles, which explains the reflection and transmission results. In this case the photons merely rattle around without losing very much energy and then leak.

These results indicate that the effect of the scattering function is appreciable when Compton scattering is important. For example, if you have an object that contains a lot of hydrogen, like your body, and you want to predict what will appear on a x-ray plate after transmission through the hydrogen, the above difference in the transmission indicates that it is important to include the scattering function in your calculations.

Coherent Scattering

Fig. 18 summarizes the effect of anomalous scattering on the coherent cross section. This effect is important at low energies and extends up to several times the K edge energy, i.e., about 1 MeV in high Z elements. Without anomalous scattering, the coherent scattering approaches a constant value at low energy. With anomalous scattering it approaches the correct zero limit as E^2 at low energy. In uranium the difference at 10 eV is about 5600 barns without anomalous scattering and 10 barns with it (a factor of 560 difference). Near photoelectric edges, anomalous scattering causes a significant decrease in the coherent cross sections, which leads to lowering of the cross sections just below the edges, allowing increased transport of photons. Since the effect of anomalous scattering has been included in the Epic coherent cross sections, we need not explicitly consider the effect further in applications, i.e., the effect is automatically included. However, we do have to consider the effect of the form factor on the angular distribution of coherently scattered photons.

For Rayleigh (coherent) scattering, compared to only using the Thomson formula, the form factor causes photons to scatter through smaller angles (more forward peaked scattering), which causes photons to transport further in their initial direction of travel. Coherent scattering is never the largest cross section, but it can have a significant effect in high Z elements just below the K edge, where it is about 10 % of the total cross section.

The following example uses 0.254 cm of lead at 11.72 grams/cc, with 80 keV photons incident (just below the lead K edge). The Epicp option to turn the form factor on or off has been used. When the form factor is turned off the cross sections calculated using the form factor are still used, but the form factor is not used the calculate the angular distribution of scattered photons; only the Thomson formula is used. In this case compared to the results without the form factor, using the form factor increases transmission by about 25 %, and decreases the reflection by more than a factor of two. These results are consistent with our expectations, since the form factor causes photons to scatter through smaller angles, continue to transport forward, and increase transmission.

Generally considering coherent scattering and ignoring the form factor is a very poor approximation. At higher energies the factor form makes coherent scattering so forward peaked, that a better approximation than using the coherent cross section and ignoring the form factor, is to completely ignore coherent scattering, i.e., set the coherent cross section equal to zero. I am merely pointing this out; I am not recommending it.

Spatial Dependence

In discussing the effect of the scattering function and form factor we have only considered integral results, i.e., deposition, reflection, transmission. Even in the cases where the overall deposition has not changed, the differences that we can see in reflection and transmission indicate that the spatial distribution of the deposition has changed. In the example lead case described above even though the overall deposition is about the same, if you are interested in the deposition half way through the lead, with the form factor the deposition is about 15 % higher.

Multi-Group Calculations

Above I have only discussed Monte Carlo, but it is worth noting that the Epic photon data base can also be used in multi-group calculations. Both the Epic data used here and the ENDF/B-VI data are based on the Livermore EPDL data. The tabulated linearly interpolable Epic cross sections are easier to use than the ENDF/B-VI formatted data to define multi-group averages. The analytical forms for coherent and incoherent scattering and fluorescence can be easily used to define group to group transfer matrices. In the case of scattering, the results should be identical to those obtained using the ENDF/B-VI data. In the case of fluorescence, Epic contains more detail than allowed in the ENDF/B-VI formats.

What's next?

As far as qualitative results, the above examples illustrate the relative importance of how cross sections are represented, fluorescence, scattering functions, form factors and anomalous scattering factors. These results should be treated only as qualitative, not quantitative results that can simulate real physical situations. The conclusions reached as far as the importance of each effect are valid, but the absolute values of deposition, transmission, etc., should be taken with a grain of salt until the calculations are performed in more detail. This is because in this paper I have only looked at one portion of the picture of photon transport. The effects of electron and positron transport must be considered in order to complete the picture.

For example, if a 20 MeV photon undergoes a pair production event, the simplest assumption is that eventually the positron will come to rest and annihilate, creating two 0.511 MeV photons. But we should ask: of the initial 20 MeV we got back about 1 MeV of energy in the form of our two 0.511 MeV photons. What happened to the other 19 MeV? Similarly, if a 20 MeV photon undergoes an incoherent scatter it can lose up to almost 99% of its energy. We can continue tracking the scattered photon, but what happened to the 99% of the energy?

The most common assumption used in many photon transport codes is that any energy lost by the photons is deposited locally at the point where each event takes place. In fact, none of the processes that I have discussed in this paper allow photons to directly deposit energy; all that photons can do is transfer their energy to electrons and positrons. So that the proper way to answer the questions that I asked above is to consider what happens to the electrons and positrons that receive energy from photons. In the case of a 20 MeV pair production, do the electron and positron really stop and deposit all of their energy very close to where the pair production occurred, or do they travel and maybe even escape from the medium? The same

should be asked of electrons that receive energy from incoherent scattering events. What about feedback? Is it important to consider bremsstrahlung, that will create more photons? What about electron ionization, that can lead to fluorescence?

I am not going to even try to cover this topic here. That's what I will cover next: A Simple Model of Electron Transport.

Conclusions

In this paper I described a simple model of photon transport. This simple model includes: tabulated cross sections and average expected energy losses for all elements between hydrogen (Z = 1) and fermium (Z = 100) over the energy range 10 eV to 1 GeV, simple models to analytically describe coherent and incoherent scattering, and a simple model to describe fluorescence. This is all of the data that is required to perform photon transport calculations.

Each of these simple models was first described in detail. Then example results are presented to illustrate the accuracy and importance of each model.

These models have now been implemented in the Epic (Electron Photon Interaction Code). All of the figures and results presented here are from Epicshow, an interactive program to allow access to the Epic data bases, and Epicp, a simple photon transport code designed to develop optimum algorithms for later use in Epic. All of the data described in this paper and all of the programs needed to use it, are available from the author.

Throughout the paper, I have tried to define where various models are important: fluorescence and scattering function at low energy, form factor at high energy. I have also tried to define guidelines as to where various models can often be ignored, e.g., the scattering function at high energy. Here, I will present a somewhat different viewpoint. Where these models are unimportant, the events that use them are highly unlikely. For example, at high energy the photoelectric cross section is so much smaller than the other cross sections, that the probability of a photoelectric event is highly unlikely; therefore, so is fluorescence. The same is true at high energy for coherent scattering. Since these events are highly unlikely, whether they are treated exactly or using an approximation will not have a significant effect on running time. When a fixed energy grid is used it is adequate for most applications, and can decrease running time for complicated problems, but it may or may not give accurate answers for any specific application.

Photons are quite different from neutrons, electrons, positrons and charged particles, in that in all elements, at all energies, the expected energy loss due to even one event is a significant fraction of the photon's energy. Photons do not have many collisions or events before they "disappear." Unlike other particles that undergo many events, each of which may have little effect on the overall history of the particles, for photons each and every event can have a major impact on a history. Therefore, care has to be used to model each and every event as accurately as possible if we are to expect accurate answers in as many different applications as possible.

The bottom line is: can you afford to have a transport code that works for most applications - but may not work for the specific applications that you are interested in. Using a fixed energy grid

can reduce running, but most other approximations discussed here have little effect on running time, but may prevent a code from giving accurate answers in certain applications - certain applications that the user will not be able to predict in advance nor be able to recognize the answers to be inaccurate. When we look at efficiency and even running time the real bottom, bottom line is Howerton's first theorem: "We are in no rush for the wrong answer" [11].

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Table Captions

1) Example Epic Tabulated Photon Data

Figure Captions

1) Comparison of EPDL and Fit Form Factor
2) Comparison of EPDL and Fit Form Factor
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